Int J Life Cycle Assess (2012) 17:350–361
DOI 10.1007/s11367-011-0364-9

UNCERTAINTIES IN LCA

On the use of possibility theory in uncertainty analysis of life cycle inventory

Jorge C. S. André · Daniela R. Lopes

Received: 22 January 2010 / Accepted: 24 November 2011 / Published online: 20 December 2011

Abstract

Purpose The purpose of this paper is to enhance the mathematical and physical understanding of practitioners of uncertainty analysis of life cycle inventory (LCI), on the application of possibility theory. The main questions dealt with are (1) clear definition of the terms—"necessity–possibility," "probability," "belief–plausibility," and of their mutual relationships; (2) what justifies the substitution of classical probability for possibility; (3) mutual comparison of, and transformations in both senses between probability and possibility uncertainty measures; (4) how to construct meaningful input possibility measures from available probabilistic/statistic information; and (5) comparative analysis of the solutions of the problem of data uncertainty propagation in LCI, afforded, respectively, by probabilistic Monte Carlo simulation and possibilistic fuzzy interval arithmetic.

Methods The questions above are addressed from the rigorous mathematical formulations of the theories of probability and statistics, of possibility, and of random sets and belief/plausibility functions, although directed to LCI uncertainty analysis practitioners. On this respect, the paper allows two different levels of reading: a basic level (main text) and a deeper level (Electronic supplementary material). Particular tools used are (a) various transformations between possibility and probability distributions, in both senses, for the continuous case, proposed by Dubois et al. (e.g., Reliable Comp 10:273-297, 2004); (b) Monte Carlo simulation for either independent or dependent input random variables; (c) fuzzy interval arithmetic; and (d) Heijungs and Suh's (2002) matrix formulation of LCI problems.

Results and discussion The links among uncertainty measures, uncertain variables, and uncertainty analysis are cleared up. It is recalled how a probability measure can be constructed and attached to an input variable, and its probability distribution and unknown "correct value" be related, in a physically meaningful way. It is justified that, usually, a dual necessity–possibility measure has much less uncertainty information than a comparable probability measure. Although the specialists are not unanimous, it is opined that the theoretical framework developed by Dubois et al. (e.g., Reliable Comp 10:273-297, 2004) is the most convenient one to use in uncertainty analysis, to compare and mutually transform probability and possibility data. This is exemplified in (a) the transformation of the very common triangular possibility and normal standard probability distributions; (b) the general construction of possibility measures from different probability data previously available; and, above all, (c) the comparison of the output information of possibilistic and probabilistic uncertainty analyses of an LCI problem proposed by Tan (Int J Life Cycle Assess 13:585–592, 2008). The general problem of data uncertainty propagation through deterministic models (e.g., of LCI) is tackled with (1) classical probabilistic Monte Carlo simulation (for either independent or dependent input random variables); (2) possibilistic fuzzy interval arithmetic; and (3) hybrid methods (only mentioned).

Conclusions (1) The practical conditions in which an analysis of uncertainty should switch from a probability to a possibility basis are still ill-defined, but that seems to be the case when the input information is based on states of large

Responsible editor: Andreas Ciroth

Electronic supplementary material The online version of this article (doi:10.1007/s11367-011-0364-9) contains supplementary material, which is available to authorized users.

J. C. S. André (✉) · D. R. Lopes
Department of Mechanical Engineering,
Faculty of Sciences and Technology, University of Coimbra,
Rua Luís Reis Santos, Pinhal de Marrocos,
3030-788 Coimbra, Portugal
e-mail: jorge.andre@dem.uc.pt

ignorance. (2) A dual necessity–possibility uncertainty measure can be viewed both as an imprecise probability measure that substitutes a definite probability for an interval, and as a belief–plausibility measure. (3) A possibility distribution can be mathematically and physically interpreted as a random set of nested prediction/confidence intervals for the "correct value" of the variable, with confidence levels ranging from 0 to 1. (4) There exist mathematically and physically sound rules to compare/transform probability and possibility uncertainty information under different applicable paradigms (e.g., based on the reliability of the input information). (5) Sometimes, Geer and Klir's (Int J Gen Syst 20:143–176, 1992) confidence index has a physically counterintuitive behavior in uncertainty analysis. (6) The probabilistic Monte Carlo simulation can be used also for dependent random input variables, only requiring more exigent input information (conditional probability distributions) than in the case of independency. (7) The possibilistic fuzzy interval arithmetic uncertainty analysis, although computationally cheap, generates output information quite poor—a good point estimate but a set of (roughly) confidence intervals with very large amplitudes for the "correct value" of each output variable.

Recommendations (1) In probability uncertainty analysis, pay attention to the relation between the "correct value" of a random variable and the parameters of its probability distribution (e.g., mean or mode). (2) Do not precipitate in changing from probabilistic to possibilistic uncertainty analysis: it may be theoretically unjustified and much output uncertainty information is lost. (3) Respect the well-established applicable rules in going from probability to possibility uncertainty information, or vice versa. (4) Be attentive to possible counterintuitive physical meaning of Geer and Klir's (Int J Gen Syst 20:143–176, 1992) confidence index in possibilistic uncertainty analysis.

Keywords Belief–plausibility measures · Fuzzy · Interval arithmetic · Monte Carlo simulation · Necessity–possibility measures · Probability–possibility transformations

1 Introduction

The need to or the interest in performing uncertainty analysis of life cycle inventory (LCI) is well known and does not require justification at this time (e.g., Lloyd and Ries 2007; Reap et al. 2008a, b).

The most informative tools of data uncertainty analysis supply interval estimates for the "correct values" of the output variables of interest, with quantitative measures of uncertainty attached. Classically, the "uncertainty measure" chosen is a "probability," by building up the uncertainty analysis upon the mathematical theory of probability and statistics (e.g., Peters 2007). However, recently, an alternative "possibility measure" is being proposed by some authors (e.g., Geldermann et al. 2000; Tan et al. 2002; Benetto et al. 2006; Tan 2008), which is defined in the theory of possibility, itself a relatively modern mathematical theory (Zadeh 1978; Dubois and Prade 1988), with clear though subtle and easily misleading relations with other modern mathematical theories of fuzzy sets (Zadeh 1965), random sets and belief/plausibility functions (Shafer 1976), and, of course, the old theory of probability and statistics. This paper intends to enhance the mathematical understanding and contextual physical interpretation of these theories in uncertainty analysis of LCI. It is directed both to soft (main text) and deep (see Electronic supplementary material) practitioners. The authors feel particularly indebted with Dubois et al., whom publications in this field cover a practically continuous period of 30 years up to the present. In this respect, Dubois et al. (2000) deserves to be highlighted.

With the above purpose, the paper commences (Section 2) with the presentation of the general backstage LCI problem and, within it, of a specific backstage case. In Section 3, the basic relations among uncertainty measures, uncertain variables, and uncertainty analysis are set up, and an overview of subsequent Sections 4 to 7, through the formulation of the two main problems of uncertainty analysis dealt with, is given. In Section 4, it is recalled how a probability measure can be constructed and related with the distribution of a random variable, and what is the relationship between the latter and the "correct value" of the underlying physical variable. In Section 5, dual possibility–necessity measures are introduced, and it is detailed both how they can be constructed for input variables (Section 5.1) and how they should be interpreted for output variables in uncertainty analysis (Section 5.2). In Section 6, the key question about which uncertainty measure, probability or possibility, can or should be attached to a given input physical variable is answered. In Section 7, the following issues of the main problem of propagation of uncertainty from input to output variables are dealt with (1) the possibility approach of fuzzy interval arithmetic (Sections 7.1 and 7.4); (2) the probability approach of the simulation of Monte Carlo (Sections 7.2 and 7.4); (3) the comparison of both former approaches in the uncertainty analysis of the backstage case (Section 7.3); and (4) emerging mixed probability/possibility approaches (Section 7.5). In Section 8, the main conclusions are highlighted.

2 Backstage LCI problem

Let us put in the backstage the general LCI problem pertaining to an "economic system" (e.g., a plant unit) encompassing n "economic processes" that consume/produce n input/output "economic commodities" (e.g., secondary materials,

products) while extracting/emitting from/to the ambient m "environmental commodities" (e.g., raw materials, pollutants), with the following matrix formulation (Heijungs and Suh 2002):

$$\mathbf{g} = \mathbf{B} \cdot \mathbf{A}^{-1} \cdot \mathbf{f} \tag{1}$$

In the matrix Eq. 1, $\boldsymbol{A}(n \times n)$ is the "technology matrix" of the system, with general element a_{ij}=(negative/positive amount of input/output economic commodity i consumed/produced per unit "scaling level" or time of operation of the economic process j), here supposed to be invertible, which implies that the, so-called allocation problem does not arise or has already been solved out for the system; $\boldsymbol{B}(m \times n)$ is the "intervention matrix" of the system, with general element b_{kj}=(negative/positive amount of input/output environmental commodity k extracted/sent from/to the environment per unit scaling level or time of operation of the economic process j); $\boldsymbol{f}(n \times 1)$ is the "functional unit column-matrix" specified in the LCI problem, with general element f_i=(negative/positive amount of input/output economic commodity i that the system is demanded to consume/produce); and the output $\boldsymbol{g}(m \times 1)$ is the "inventory or environmental interventions column-matrix," with general element g_k=(total negative/positive amount of input/output environmental commodity k extracted/sent from/to the environment by the system).

Tan's (2008) case I will serve as a specific example (Fig. 1), heretofore named "backstage case." In this case, the system encompasses processes I and II (j=1 and 2). Both processes emit the pollutant D (environmental commodity with k=1) to the environment, but while process I consumes the product B (economic commodity with i=2) and produces the product A (economic commodity with i=1), process II does the inverse, which allows the system to operate in an economically efficient recycling mode. The technology $\boldsymbol{A}$, intervention $\boldsymbol{B}$, and functional $\boldsymbol{f}$ input matrices of the system/problem are given below (Eqs. 2a–c), with all amounts expressed in mass units of kilogram. For each one of the "uncertain input variables" (a_{11}, a_{22}, b_{11}, b_{12}), best estimates of the lower bound, point value, and upper bound of the respective (unknown) "correct value" are given. The single scalar output variable is g_1=(total amount of pollutant D emitted by the system for this to satisfy the required demand).

$$\mathbf{A} = \begin{bmatrix} (0.5, 0.6, 1) & -1 \\ -1 & (3, 5, 6) \end{bmatrix}, \mathbf{B} = [(0.05, 0.06, 0.07) \ (0.9, 1, 1.1)], \quad \mathbf{f} = \begin{bmatrix} 100 \\ 0 \end{bmatrix} \tag{2a–c}$$

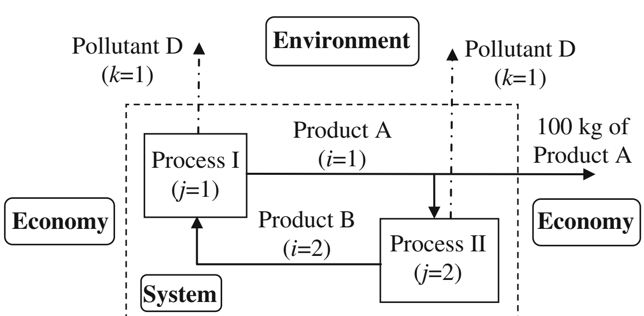

Fig. 1 Scheme of the so-called, in the paper, backstage case: Tan's (2008) case I system operating in the steady-state condition demanded. (Notice that for this condition to be physically possible, some inputs must be neglected, which does not matter here.)

3 Uncertainty measures and uncertain variables in uncertainty analysis

Any "uncertain variable" X with domain $U \subseteq \mathbb{R}$ ($\mathbb{R}$ being the mathematical set of real numbers) can be associated with an actual or virtual "non-deterministic experiment" $\boldsymbol{E}$ with set of results U, i.e., a "repeatable" experiment in which, although all relevant "deterministic" factors are directly or indirectly controlled, the value $x \in U$ taken by X in any individual realization of $\boldsymbol{E}$ (in uncertainty analysis, usually, x is the outcome of a measurement procedure specified in $\boldsymbol{E}$) cannot be predicted deterministically in a reliable way (e.g., André 2008). In any realization of $\boldsymbol{E}$, if its result is $x \in A$ then "event" A is said to have occurred, and $\mathrm{M}(A) \in [0, 1]$ is the general designation of a quantitative measure of the experimenter's (un)certainty that A will actually occur. For instance, for the variable $X \equiv a_{11}$ of the backstage case (Section 2) and the event A=[0.5, 1], whatever measure M is adopted, one would expect that $\mathrm{M}(A)$=1.

The first problem the uncertainty analysis tools dealt with in this paper must solve is to choose an appropriate uncertainty measure M connected with each uncertain variable X and respective non-deterministic experiment $\boldsymbol{E}$ with set of results U. Two main alternative solutions to this problem are considered here: either a probability measure P (Section 4) or a dual necessity–possibility measure N-Π (Section 5), both defined in U. The choice between both is discussed in Section 6.

The second problem the uncertainty analysis must solve is the propagation of uncertainty from input to output variables, i.e., "Given: n uncertain input variables (X_1, X_2, …, X_n) with known uncertainty distributions, and an output variable Y related with the former input variables through a known deterministic function Y=h(X_1, X_2, …, X_n); obtain: the uncertainty distribution of Y." Consistently with the first problem, some or all the input variables can be probabilistic or random variables and, the remaining ones, possibilistic or fuzzy variables. Besides, different probabilistic/possibilistic relations may exist among the input variables, ranging from

simple independence to different types and degrees of correlation. This problem is dealt with in Section 7.

4 Probability uncertainty measures and random variables

As a sound foundation of the mathematical theory of probability and statistics, Kolmogorov (1950) defined a "probability measure" P in a universe set U, by associating to (almost) any subset A of U, a number P(A), satisfying the following three axioms: (A1) P(A)≥0, (A2) P(U)=1, and (A3) (additivity axiom for two sets) if $A \cap B = \varnothing$, then P($A \cup B$)=P(A)+P(B).

To attach a probability measure P (in U) to a given uncertain physical variable X with domain $U \subseteq \mathbb{R}$, in a physically meaningful way, it is required, in the first place, that X be a "random variable," i.e., that the non-deterministic experiment $\boldsymbol{E}$ behind X falls into the restrict class of "random experiments."

In the second place, the measure of probability P linked to the random experiment $\boldsymbol{E}$ with set of results U can be constructed from scratch through mainly three methods (André 2008)—method 1 (Empirical Method): to perform $\boldsymbol{E}$ as many times as possible ($n \to \infty$) and to rely upon the asymptotic identity: $P(A) = \lim_{n \to \infty} f_n(A)/n$, where $f_n(A)$= (number of occurrences of A in the first n realizations of $\boldsymbol{E}$); method 2 (Theoretical Method): if U is finite and the physical "hypothesis of symmetry" according to which "all results r in U are equally likely" is applicable, then P(A)=n(A)/n(U), where $n(\cdot)$≡"number of elements of;" and method 3 (Subjective Method): P(A)=(subjective estimate of an "expert"). It is important to understand that each one of these methods has its own non-mathematical conditions of correct application. For instance, in method 1, problems with the control of experiment $\boldsymbol{E}$ can be detected through the apparent divergence of the succession $p_n = f_n(A)/n$, and, in method 3, the choice of the "expert" can be very relevant. Besides, if all methods fail to give any or mutually consistent results, then, the possibility that the experiment $\boldsymbol{E}$ is intrinsically "non-random" should be considered (cf. Section 6).

In the third place, the relation between the probability measure P attached to ($\boldsymbol{E}$, U) and the probability function p: $U \to [0,1]$ of the random variable X, if X is discrete, or the probability density function f of X, f:$U \to [0,+\infty[$, if X is continuous, is, respectively:

$$P(A) = \sum_{x \in A} p(x) \text{ or } \int_{x \in A} f(x) \cdot dx \tag{3a, b}$$

Finally, in the fourth place, in uncertainty analysis, denoting by x^* the "correct value" of X, if its measurement procedure is "non-biased" (in average), then $x^* = \mu$, μ being the probabilistic mean of X. Furthermore, if the probability distribution of X is symmetrical and unimodal then it is also $x^* = \mu = x_0$, x_0 being the "mode" of X. Both the former conditions apply to many physical random variables. However, non-symmetrical lognormal probability distributions are assumed for the variables of all unit processes in ecoinvent data v1.1 (Frischknecht et al. 2005). Moreover, when X is measured indirectly through other basic random variables (X_1, X_2, …, X_m) with which it bears the deterministic relationship $X = h(X_1, X_2, \ldots, X_m)$, if h is non-linear and the standard deviations of the basic variables are not all small, the distribution of X will be biased and asymmetrical, even if the distributions of the basic variables are non-biased and symmetrical, i.e., $x^* = h({x^*}_1, {x^*}_2, \ldots, {x^*}_m) \neq \mu$, x_0 even if ${x^*}_i = \mu_i = x_{0i}$ (i=1, 2, …, m).

5 Possibility uncertainty measures and possibilistic or fuzzy variables

In the theory of possibility (Schackle 1961; Zadeh 1978; Dubois and Prade 1988), a "possibility measure" Π is defined in the universe set U by associating to any subset $A \subseteq U$ a number Π(A) satisfying the following axioms (Dubois et al. 2000): (A1′) Π(∅)=0; (A2′) Π(U)=1 (normal case); and (A3′) (maxitivity axiom) for any A, $B \subseteq U$, Π($A \cup B$)=max{Π(A), Π(B)} (cf. the additivity axiom A3 in Section 4).

If $U \subseteq \mathbb{R}$, the possibility measure Π can be associated with a "possibilistic or fuzzy variable" X characterized by the "possibility distribution" $\pi : \mathbb{R} \to [0,1]$, such that:

$$\Pi(A) = \sup\{\pi(x), x \in A\}, \tag{4}$$

with $\pi(x)$=1 for one (and only one, the mode x_0, if π is unimodal, as is most usual) or more values $x \in \mathbb{R}$. The possibility measure Π has also associated to it the dual "necessity measure" N defined, in this way:

$$N(A) = 1 - \Pi(\overline{A}) \tag{5a}$$

It is simple to show that (Dubois 2006):

$$N(A) = \inf\{1 - \pi(x), x \in \overline{A}\} \text{ and } \qquad N(A \cap B) = \min\{\mathrm{N}(A),\ \mathrm{N}(B)\} \tag{5b, c}$$

The identity Eq. 5c is called the minitivity axiom for the necessity measure (cf. the maxitivity axiom A3′ above). Figure 2 illustrates the definition of the dual measure Π-N for a generic unimodal possibility distribution π.

5.1 Construction of possibility measures for input variables

Due to the relative youth of possibility theory (Zadeh 1978), the empirical procedures and physical hypotheses and ideas available to directly construct the possibility measure Π

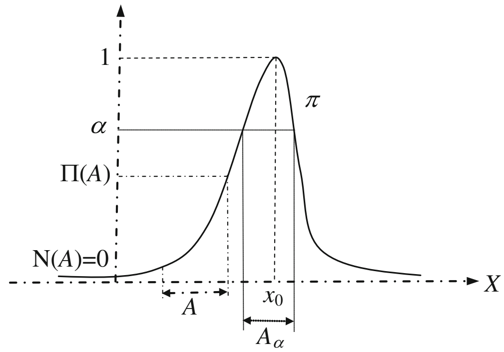

Fig. 2 Definition of the dual possibility–necessity measure Π-N associated with the possibilistic or fuzzy variable X with unimodal possibility distribution π with mode x_0, for a generic event A. The event A_α is called the "α-cut of π". Per definition, irrespective of α, $\Pi(A_\alpha)=1$ and $N(A_\alpha)=1-\alpha$

attached to a physical input variable X are not so well understood as the ones behind the methods 1–3 that are used to construct probability measures (cf. Section 4). They are not reviewed here but the interested reader can consult, e.g., Hersh and Caramazza (1976), Hisdal (1991), and Tong et al. (2004). Instead, three useful indirect methods of construction of physically meaningful possibility measures are proposed below. In a more (methods I–II) or less (method III) extent, all methods start from a given probability measure P (here X is still envisaged as a random variable) and afford, through an appropriate transformation Π=T(P), the "nearest" possibility measure Π (X is now seen as a possibilistic variable), in a certain sense. A basic hypothesis shared by the three methods, with the exception of the final variant of method III (triangular possibility distributions), consists in supposing that, for unimodal probability distributions P, the mode x_0 is the best point estimate $\widehat{x}^*$ of the "correct value" x^* of the physical variable behind X. In fact, if P is asymmetric then, most commonly, $x^*=\mu\neq x_0$ (cf. Section 4, in fine). However, in these cases, it seems that a possible way around could be to translate the probability distribution P of X in order to enforce that $x_0=\widehat{x}^*$. The underlying theory is covered in Section A2.2 of the Electronic supplementary material for the interested reader, where the rationale behind some symbology is also given.

Method I A sound probability measure P is available for X, typically obtained with the method 1 (empirical) of Section 4. Here, we consider only the case of a continuous random variable X with unimodal probability density function f with mode x_0, strictly increasing for $x<x_0$ and strictly decreasing for $x>x_0$. In this case, the possibility distribution π of X should be obtained by applying to f the following transformation $\pi=T_2(f)$:

$$\pi(x)=\pi(y)=F(x)+1-F(y) \text{ for } x\leq x_0, y\geq x_0 \text{ and } f(y)=f(x) \qquad (6a, b)$$

In Eqs. 6a, b: F is the distribution function of variable X; and the interval $[x, y]$ can be interpreted as the $f(x)$-cut of f, i.e., the analogue of the α-cut A_α of π (cf. Fig. 2).

Method II A probability distribution P much less reliable than the one of method I, typically obtained with method 3 (subjective) of Section 4, is available for X. Now, for a continuous random variable X with probability density function f, the transformation to apply is $\pi=T_1^{-1}(f)$:

$$\pi(x)=\int_{x'\in U}\min\{f(x),f(x')\}\cdot dx' \text{ for any } x\in U \qquad (7)$$

In Fig. 3, the possibility distribution π_1 resulting from the application of T_1^{-1} to a normal standard random variable X can be compared with the possibility distribution π_2 obtained by method I for the same case.

Method III The uncertainty information available on X is a set of reliable prediction intervals $\widehat{i}^*_{\alpha'}$ ($\alpha'=\alpha'_1$, …, α'_p) of estimation (either empirical or subjective) of the "correct value" x^* of X, for some confidence levels $\alpha'\in[0,1]$. In particular, for $\alpha'=0$ the prediction interval collapses into a simple point estimate: $\widehat{i}^*_0\equiv\widehat{x}^*$. If the prediction intervals (for $\alpha'>0$) are classical statistics confidence intervals obtained from an empirical sample of X, for unimodal probability distributions P of X (in this case, unknown in detail), an estimator for the mode should be used and the sample must also be one-dimensional (i.e., have a single value). In any case (postulating also that π is unimodal with mode x_0, increasing for $x<x_0$ and decreasing for $x>x_0$), the same transformation T_2 of method I can be applied to each prediction interval $\widehat{i}^*_{\alpha'}=\left[\widehat{x}_{m,\alpha'},\widehat{x}_{M,\alpha'}\right]$, which leads to the simple identities:

$$\pi\left(\widehat{x}_{m,\alpha'}\right)=\pi\left(\widehat{x}_{M,\alpha'}\right)=1-\alpha' \qquad (8a, b)$$

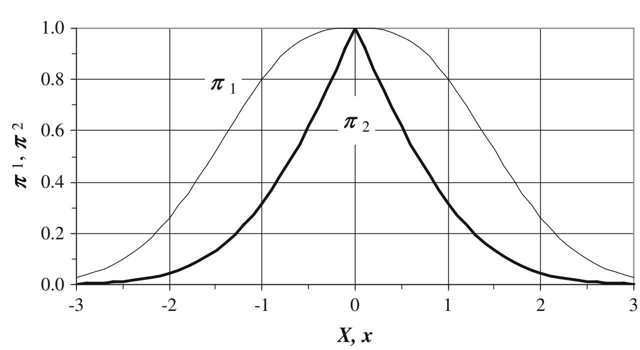

Fig. 3 Possibility distributions $\pi_2=T_2(f)$ and $\pi_1=T_1^{-1}(f)$ obtained for X (envisaged as a possibilistic or fuzzy variable) from a previously available normal standard probability density function f of X (envisaged as a random variable), respectively, by methods I and II. In both cases, $x_0=0$ is the best available point estimate of the "correct value" x^* of the physical variable behind X

In particular, for α'=0, Eqs. 8a, b further collapse into:

$$\pi(\widehat{x}^*) = 1 \tag{8c}$$

The possibility distribution $\pi(x)$ can be guessed in the rest of U with an appropriate best fitting procedure of the set of points $\{(\widehat{x}_{m,\alpha'}, \pi(\widehat{x}_{m,\alpha'}))$, $(\widehat{x}_{M,\alpha'}, \pi(\widehat{x}_{M,\alpha'}))$ for $\alpha'=\alpha'_1, \ldots, \alpha'_p\}$. In the often case in which the only available information on X is $\widehat{x}^*$ and $\widehat{i}^*_1 = [\widehat{x}_{m,1}, \widehat{x}_{M,1}]$, it is a good option to take a triangular possibility distribution π for X, with mode $x_0 = \widehat{x}^*$ and support $[x_m, x_M]=\widehat{i}^*_1$ (e.g., the possibility distribution π in Fig. 4), as justified in Section A3 of the Electronic supplementary material.

5.2 Physical interpretation of possibility measures of output variables

Let us now suppose that the pertinent uncertainty propagation problem formulated in general terms in Section 3 and dealt with in depth in Section 7 has already been solved, affording the possibility distribution π of the possibilistic output variable $Y=h(X_1, X_2, \ldots, X_n)$. How should the uncertainty information inherent to π be interpreted? To simplify without significant loss of practical generality, when not mentioned otherwise, π is supposed to be unimodal with mode y_0. Besides, consistently with Section 5.1, it is presupposed that the mode x_{0i} of the possibility distribution π_i of input variable X_i (i=1, 2, …, n) is the best available point estimate of its "correct value" x_i^*, i.e., $\widehat{x}_i^* = x_{0_i}$.

In the first place, the mode y_0 is the best available point estimate of the "correct value" y^* of the physical variable behind Y, namely, $y_0 = \widehat{y}^* = h(\widehat{x}^*_1, \widehat{x}^*_2, \ldots, \widehat{x}^*_n)$.

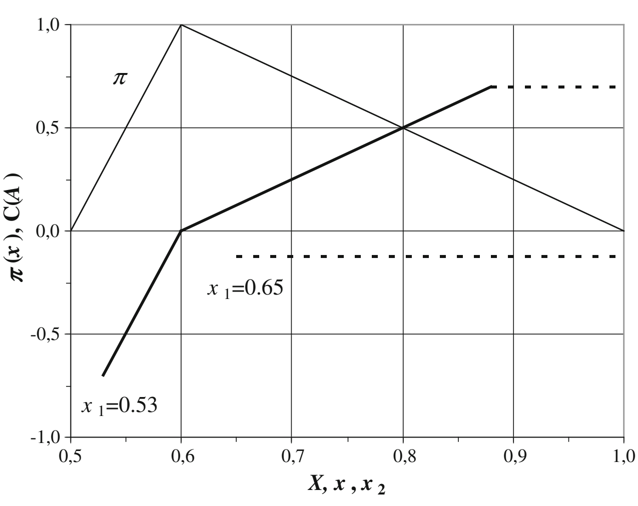

Fig. 4 Geer and Klir's (1992) "confidence index" C(A) (*thick lines*) in events $A=[x_1,x_2]\subseteq U$, x_1 and x_2 being, respectively, fixed and free parameters, for a fuzzy variable X with triangular possibility distribution π with support U=[0.5,1] and mode x_0=0.6 (*thin line*). Positive/negative values of C(A) are said to confirm/disconfirm event A but, in the case of interrupted lines, this interpretation of C(A) is counterintuitive

In the second place, and this is the deepest applicable theoretical result, the α-cut A_α of the possibility distribution π (see Fig. 2) can be roughly interpreted as a "confidence interval" $\widehat{i}^*_{\alpha'}$ of estimation of y^* with confidence level $\alpha'=1-\alpha$, as the latter is defined in classical statistics theory for a single-value sample. However, depending on π, the amplitude of $\widehat{i}^*_{\alpha'}$ can be much larger than the amplitude of the optimum (i.e., narrowest) confidence interval with level α'. For instance, due to an optimal property of transformation T_2, the α-cut of the possibility distribution π_2 of X represented in Fig. 3 is the narrowest confidence interval for x^* with confidence level $\alpha'=1-\alpha$, and, in this sense, π_2 has much more uncertainty information than π_1. The theory underlying this result is given in Sections A2.2 and A4 of the Electronic supplementary material (see also: Yager 1992, Smets 1990, Dubois et al. 2008).

Finally, in the third place, the following "confidence index (in event A)" C(A)∈[−1,1] of Geer and Klir (1992) is sometimes (e.g., Benetto et al. 2006) used to synthesize the uncertainty information contained in a dual possibility–necessity measure Π-N:

$$C(A) = \Pi(A) + N(A) - 1 = \Pi(A) - \Pi(\overline{A}) \tag{9a, b}$$

Specifically, positive/negative values of C(A) are interpreted as "degrees of confirmation/disconfirmation" of A. However, this interpretation of C(A) can sometimes be counter intuitive. For instance, in the case of a simple triangular possibility distribution π with support U=[0.5,1] and mode x_0=0.6 (see Fig. 4), for the family of events $A=[0.53,x_2]$, C(A) keeps a constant value of 0.7 for increasing x_2 above 0.88, while, by physical sense (perhaps, induced by probabilistic thinking), one would expect that it continued to approach 1. In fact, the maximum degree of confirmation C(A)=1 is only attained if, and only if, the event $\overline{A}$ is impossible, with Π(A)=1 and Π($\overline{A}$)=0, while, for the former family of events A, no matter how large is x_2, it is always Π($\overline{A}$)≥π(0.53)=0.3>0.

6 The choice between probability and possibility uncertainty measures

Let us commence by clearing up a basic question. Although Klir and Parvis (1992) (see Klir 2006 for a more recent presentation) say that (in a given universe set U) there exist measures of possibility–necessity Π-N and of probability P that are "commensurate," i.e., that have essentially the same uncertainty information, the authors follow Dubois et al., who defend convincingly that the former is always "weaker," i.e., it has less precise uncertainty information, than a comparable probability measure (e.g., Dubois et al. 1993, 2000; Dubois 2006). Their arguments are reviewed in

Section A1 of Electronic supplementary material (see also: Walley 1991, Giles 1982, De Cooman and Ayels 1999).

The main question dealt with in this section is the following one: Given an input physical variable X associated with the non-deterministic experiment $\boldsymbol{E}$, should the uncertainty inherent to the determination of its "correct value" x^* be quantified through a probability measure P or through a dual possibility–necessity Π-N measure? In other words, should X be treated as a random variable or as a possibilistic/fuzzy variable?

At the onset, two circumstances may dictate the convenience of preferring a possibility to a probability measure for X: (1) only method 3 of Section 4 (subjective estimates of experts) can be used to construct the probability measure and the available experts are largely ignorant on the outcomes of experiment $\boldsymbol{E}$; and (2) it is wished to reduce the computation time of resolution of the subsequent uncertainty propagation problem. Regarding case 1, notice that an expert totally ignorant about event A (in $\boldsymbol{E}$) could consistently postulate that $\Pi(A)=\Pi(\overline{A})=1$ and $N(A)=N(\overline{A})=0$ (cf. Section 5) but if it postulates, for instance, that $P(A)=0.8$ then it must consistently postulate that $P(\overline{A})=1-P(A)=0.2$ (cf. axioms A1–3 of Section 4). Similarly, the so called "vacuous possibility measure," according to which $\Pi(A)=1$ for any $A\subseteq U$, is much less informative than the analogous "uniform probability measure" (Dubois 2006). In Section A1 (Electronic supplementary material), it is explained in more detail why possibility theory is a theoretical frame more adequate than probability and statistics theory to deal with uncertainty under states of large ignorance. Case 2 is discussed in Section 7.3.

If the former circumstances simply do not occur or are not determinant, a random experiment $\boldsymbol{E}$ can be assumed and any of the methods 1–3 of Section 4 used to construct a probability measure P attached to X, or, what is equivalent, a probability distribution for X. In this process, two other circumstances, and none more the authors can think of, can still lead to the mandatory substitution of the probability model by a possibility model: (3) in the course of the application of method 1, $\boldsymbol{E}$ is suspected to be non-random, or (4) while applying method 3, independent estimates of the probabilities of a set of interconnected events (e.g., A, B, $A\cap B$ and $A\cup B$), supplied by one or more experts, lead to a gross violation of axioms A1–3 (Section 4). The possibility of case 3 is already foreseen in Section 4. On case 4, Dubois (2006) mentions a study of Raufaste et al. (2003) that would suggest that subjective estimates of uncertainty measures tend to obey the maxitivity/minitivity axiom (A3′) of possibility theory rather than the additivity axiom (A3) of probability theory. Taking the example given above within parenthesis, to postulate that $P(A)=0.2$, $P(B)=0.4$, $P(A\cap B)=0.1$ but $P(A\cup B)=0.3$ is inconsistent with axioms (A1–3) because they imply that $P(A\cup B)=P(A)+P(B)-P(A\cap B)$.

7 Uncertainty propagation problem

7.1 Possibilistic approach

Let us take once again the backstage case (cf. scheme Fig. 1 and numerical inputs Eqs. 2a–c). For each uncertain input variable X, following the last variant of method III of Section 5.1, Tan (2008) adopts a triangular possibility distribution π with support $[x_m, x_M]$ and mode x_0, where (x_m, x_0, x_M) are the best available estimates, respectively, of the lower bound, point value and upper bound of the "correct value" x^* of X (e.g., in Fig. 4 it is shown the possibility distribution π postulated for $X\equiv a_{11}[x_m=0.5, x_0=0.6, x_M=1.0]$).

For reasons and in conditions (really, still not fully understood) that are explained in Section A5 of the Electronic supplementary material (see also: Zadeh 1975a,b, Gebhardt and Kruse 1994), the solution of the uncertainty propagation problem $Y=h(X_1, X_2, \ldots, X_n)$ in possibility theory can be cast into a simple form called after "fuzzy interval arithmetic," used, namely, by Dubois et al. (2004a, b) and Tan (2008), which affords any α-cut $A_{Y,\alpha}$ ($\alpha\in[0,1]$) of the possibility distribution π of the output variable Y, in the following form:

$$A_{Y,\alpha} = \left[y'_\alpha, y''_\alpha\right], \text{with} \tag{10a}$$

$$y'_\alpha,\ y''_\alpha = \inf, \sup\left\{h(x_1, \ldots, x_n) : x_1 \in A_{X_1,\alpha} \cap \ldots \cap x_n \in A_{X_n,\alpha}\right\} \tag{10b, c}$$

In Eq. 10b,c, $A_{X_i,\alpha}$ denotes the α-cut of the possibility distribution π_i of the input variable X_i. Specifically for the general backstage LCI problem with matrix-Eq. 1, in which $Y\equiv g_k$, the following expressions can be used to explicitly solve the min–max problem posed by Eq. 10b,c:

$$g_{k,\alpha}{}', g_{k,\alpha}{}'' = \begin{cases} h\left(\ldots, a_{ij,\alpha}{}', a_{ij,\alpha}{}'', \ldots, b_{ij,\alpha}{}', b_{ij,\alpha}{}'', \ldots\right) & \text{if } \frac{\partial g_k}{\partial a_{ij}}, \frac{\partial g_k}{\partial b_{ij}} \geq 0 \\ h\left(\ldots, a_{ij,\alpha}{}'', a_{ij,\alpha}{}', \ldots, b_{ij,\alpha}{}', b_{ij,\alpha}{}'', \ldots\right) & \text{if } \frac{\partial g_k}{\partial a_{ij}} < 0 \text{ but } \frac{\partial g_k}{\partial b_{ij}} \geq 0 \\ h\left(\ldots, a_{ij,\alpha}{}', a_{ij,\alpha}{}'', \ldots, b_{ij,\alpha}{}'', b_{ij,\alpha}{}', \ldots\right) & \text{if } \frac{\partial g_k}{\partial a_{ij}} \geq 0 \text{ but } \frac{\partial g_k}{\partial b_{ij}} < 0 \\ h\left(\ldots, a_{ij,\alpha}{}'', a_{ij,\alpha}{}', \ldots, b_{ij,\alpha}{}'', b_{ij,\alpha}{}', \ldots\right) & \text{if } \frac{\partial g_k}{\partial a_{ij}}, \frac{\partial g_k}{\partial b_{ij}} < 0 \end{cases} \tag{11}$$

$$\text{with}: \frac{\partial g_k}{\partial a_{ij}} = -c_{ki} \cdot s_j \text{ and } \frac{\partial g_k}{\partial b_{ij}} = \delta_{ki} \cdot s_j \qquad (12a, b)$$

In the right members of the multiple Eq. 11: h stands for the scalar deterministic function linking the output g_k to all the inputs (a_{ij}, b_{ij}, f_i), consistent with the matrix-Eq. 1; and it is supposed that the α-cuts of the possibility distributions of the output variable g_k and of the input variables a_{ij} and b_{ij} are, respectively: $A_{g_k,\alpha} = \left[g_{k,\alpha}{}', g_{k,\alpha}{}''\right]$, $A_{a_{ij},\alpha} = \left[a_{ij,\alpha}{}', a_{ij,\alpha}{}''\right]$ and $A_{b_{ij},\alpha} = \left[b_{ij,\alpha}{}', b_{ij,\alpha}{}''\right]$. In Eq. 12a,b, which are easy to derive from Eq. 1 (Heijungs and Suh 2002), c_{ki} and s_j are the general elements of matrices, respectively, $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}^{-1}$ and $\mathbf{s} = \mathbf{A}^{-1} \cdot \mathbf{f}$, the latter also called "scaling or times column-matrix," and δ_{ki} is Krönecker's delta, i.e., δ_{ki}=0 or 1 whether $k \neq i$ or $k=i$. Unfortunately, this fast min–max algorithm may afford wrong solutions if h is strongly nonlinear on an input a_{ij} with an α-cut of large amplitude. However, further to the fact that this occurrence is supposed to be rare in practice, a more general algorithm would also be much more time consuming. On the contrary, Tan (2008) uses an even faster and simpler form of the above algorithm to solve the back-stage case, in which the signs of the partial derivatives in the right members of Eq. 11 are assumed a priori and so, Eq. 12a,b can be dispensed. The price paid is that the conditions of correct application of the algorithm become also more restrictive, as explained in Heijungs and Tan (2010).

Anyway, the result of applying fuzzy interval arithmetic to solve the uncertainty propagation problem of the back-stage case is the possibility distribution π for the output variable $Y \equiv g_1$ shown in Fig. 5, computed for 11 α-cuts evenly spaced in the range of α between 0 and 1.

7.2 Probabilistic approach for independent input variables

A general solution for the propagation problem $Y=h(X_1, X_2, \ldots, X_n)$ in probability and statistics theory, even in the simplest case of independent input variables, is not available in analytical form. However, the method of simulation of Monte Carlo affords a numerical solution in three straightforward steps (e.g., André 2008):

1. Generate independent N-dimensional random samples $A_{i,N}=(x_{i,1}, x_{i,2}, \ldots, x_{i,N})$ for each one of the input variables X_i (i=1, …, n). This step requires the availability of a uniform probability density generator in the interval [0,1], such as, the function *RAND()* of EXCEL™, and is back up on a well-known theorem of probability theory. More specifically, if $z_{i,j}$=*RAND()* and X_i is a continuous random variable with invertible distribution function F_i, then it is simply:

$$x_{i,j} = F_i^{-1}\left(z_{i,j}\right) \text{for } i = 1, 2, \ldots, n \text{ and } j = 1, 2, \ldots, N \qquad (13a)$$

2. Generate an N-dimensional sample $A_N=(y_1, y_2, \ldots, y_N)$ for the output variable Y, from the n samples $A_{i,N}$ (i=1, …, n) generated in step 1, in the following way:

$$y_j = h\left(x_{1,j}, x_{2,j}, \ldots, x_{n,j}\right) \text{for } j = 1, 2, \ldots, N \qquad (13b)$$

3. Calculate "empirically"−i.e., ultimately based on method 1 of Section 4—from the sample A_N generated in step 2, the desired probability distribution of Y (e.g., the probability density function f_Y, if Y is a continuous random variable), or any of its characteristic moments (e.g., mean μ_Y, mode y_0 or standard deviation σ_Y), with the help of appropriate sample estimators.

The numerical solutions afforded in step 3 for function f_Y or parameters (μ_Y, y_0, σ_Y) are affected by random errors with vanishing standard deviations for increasing sample dimension N. Unfortunately, to bring the values of these standard deviations below acceptable thresholds, the value of N must usually be very large, of the order $O(N) \sim 10^4 - 10^5$, which turns out the method computationally heavy, especially if the number n of input variables is large or the functions F_i^{-1} (i=1, 2, …, n) or h are, themselves, heavy to compute.

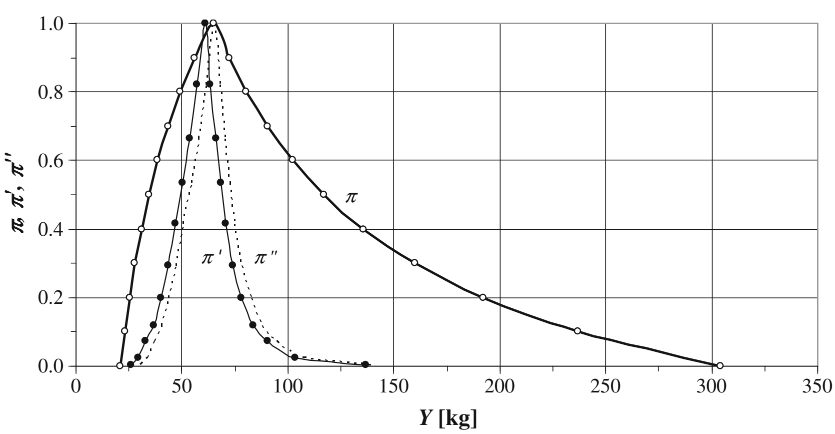

Fig. 5 Possibility distribution π (*white circles* denote calculation points) of the output variable Y [kg]$\equiv g_1$=(total amount of pollutant D emitted to the environment) that results of the possibilistic uncertainty analysis of the backstage case versus the possibility distributions π' (*black circles* denote calculation points) and π'' that result of the "most likely" probabilistic uncertainty analysis of the same case (cf. Section 7.3)

7.3 Comparison of possibilistic and probabilistic approaches for independent input variables

The analysis of the backstage case of Section 7.1 is considered illustrative of the possibilistic approach for the uncertainty propagation problem. For reasons that are explained in Section A2 of the Electronic supplementary material, the probabilistic uncertainty analysis that compares best with the former possibilistic analysis must perform the three following steps orderly:

1. To convert the triangular possibility distribution $\pi_i(x_{mi}, x_{0i}, x_{Mi})$ postulated for each uncertain input variable X_i (i=1, …, 4) (see π_1 of $X_1 \equiv a_{11}$ in Fig. 6), into the following "most likely" probability density function $f_i = T_1(\pi_i)$:

$$f_i(x) = \int_0^{\pi_i(x)} \frac{d\alpha}{\left|A_{X_i,\alpha}\right|}, \text{ for any } x \in U \tag{14}$$

In Eq. 14, $\left|A_{X_i,\alpha}\right|$ designates the amplitude of the α-cut $A_{X_i,\alpha}$ of the possibility distribution π_i. The analytic solution for f_i is (see f_1 in Fig. 6):

$$f_i(x) = -\frac{1}{x_{M_i} - x_{m_i}} \cdot \begin{cases} \ln((x_{0_i} - x)/(x_{0_i} - x_{m_i})) \text{ for } x_{m_i} \le x \le x_{0_i} \\ \ln((x - x_{0_i})/(x_{M_i} - x_{0_i})) \text{ for } x_{0_i} < x \le x_{M_i} \end{cases} \tag{15a, b}$$

2. To apply the method of simulation of Monte Carlo (Section 7.2) to the propagation problem resulting from step 1, to obtain the probability density function f_Y of the output variable Y. For this step to be taken, the distribution function F_i corresponding to f_i must firstly be obtained and, afterwards, inverted to get F_i^{-1}. The latter has no analytic expression but can be fitted with a sixth-degree polynomial across the whole support $[x_{m,i}, x_{M,i}]$ of variable X_i, with relative error smaller than 1% everywhere except, possibly, near the extremes, where it may attain 3%. Eventually, the function f_Y can be estimated with negligible random error, generating a sample with dimension $N=5\times10^4$ and partitioning the relevant part of the domain of Y into m=32 even classes.
3. To convert the probability density function f_Y obtained in step 2, into the "most likely" possibility distribution $\pi' = T_2(f_Y)$ (Eq. 6a, b; see Fig. 5).

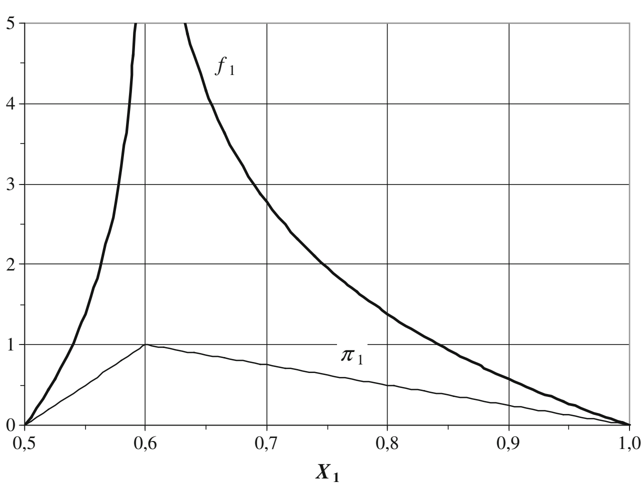

Fig. 6 Probability density function f_1 (Eq. 15a,b) "most likely" to the triangular possibility distribution π_1 of the input variable $X_1 \equiv a_{11}(x_{m1}$= 0.5, x_{01}=0.6, x_{M1}=1.0) of the backstage case

Comparing the curves of the two possibility distributions π and π' in Fig. 5, the following can be concluded: (1) the construction of π is much less time consuming than the one of π' (in this case, π required only 21 computations of the pertinent scalar function h while π' required 5×10^4); (2) the mode $y_0 = h(x_{01}, x_{02}, x_{03}, x_{04})$ of π is the best point estimate of the "correct value" y^* of the output variable Y (cf. Section 5.2), while, relative to y_0, the mode y_0' of π' is biased downwards in 6%; and (3) π' is much narrower than π (the comparison is simplified by substituting π' for $\pi''(y) = \pi'(y+\varepsilon_0)$, with $\varepsilon_0 = y_0' - y_0$, as shown in Fig. 5), which, following the interpretation given in Section 5.2, means that π' (π'') keeps much more uncertainty information than π. Notice that the bias of π' mentioned in conclusion 2, which is due to a bias of the underlying probabilistic uncertainty analysis of the type mentioned in Section 4 (in fine), does not represent any loss of uncertainty information of the probabilistic approach, as the point-estimate y_0 of y^* is not an exclusive of the possibilistic approach. Specifically, the narrowest confidence/prediction interval $\widehat{i}^*_{\alpha'}$ for y^*, with any desired confidence level $\alpha' \in [0,1]$, that can be obtained from (f_Y, y_0), is simply the α-cut of the translated possibility distribution π'' (see above) for $\alpha = 1-\alpha'$.

Summing up, the price paid by the possibilistic approach for being so light-computing is the poverty of its output uncertainty information (the possibility distribution π) on Y, which consists: (1) in the mode y_0 of π, which is, in fact, a good point-estimate of the "correct value" y^*; but (2) for any other α-cut of π with $\alpha<1$, in "confidence intervals" for y^* with confidence levels $\alpha' = 1-\alpha$ but amplitudes much larger than the optimum (compare the amplitudes of the α-cuts of π and π'' in Fig. 5). On the contrary, the probability approach, despite being much more time consuming, affords a probability distribution for Y that contains much richer output uncertainty information on Y.

7.4 Probabilistic and possibilistic approaches for correlated input variables

When the random input variables X_i are mutually dependent or correlated, the step 1 of the probabilistic method of simulation of Monte Carlo of Section 7.2 is readily

adaptable to cope with it. Take, for instance, the case of three dependent input continuous random variables, X_1, X_2, and X_3. Further to the usual marginal distribution function $F_1(x_1)$ of X_1, the method now requires, as input, instead of the usual marginal (1D) distribution functions $F_2(x_2)$ of X_2 and $F_3(x_3)$ of X_3, the conditional (respectively, 2D and 3D) distribution functions $F_{2|1}(x_2|x_1)$ and $F_{3|1\cap 2}(x_3|x_1,x_2)$, which only collapse into $F_2(x_2)$ and $F_3(x_3)$, respectively, when the variables X_1, X_2 and X_3 are mutually independent. Afterwards, the sample $A_{1,N}$ is generated firstly, as usual, with Eq. 13a, but the samples $A_{2,N}$ and $A_{3,N}$ must be subsequently generated, the latter after the former, thus:

$$x_{2,j} = F_{2|1}{}^{-1}\left(z_{2,j}|x_{1,j}\right) \text{ and } x_{3,j} = F_{3|1\cap 2}{}^{-1}\left(z_{3,j}|x_{1,j}, x_{2,j}\right) \quad (16a, b)$$

So, the method of simulation of Monte Carlo has no limitations of principle to deal with correlated input variables, and does not even become computationally heavier, the only problem being that it now requires more, and also more complex to obtain, input probabilistic information than in the case of independent input variables.

On the contrary, the fuzzy interval arithmetic of Section 7.1 not only does not require any modification to be able to cope with dependent possibilistic input variables but, as long as they depend on a common source of information (see Section A5 of the Electronic supplementary material and also Gebhardt and Kruse 1994) does not even require any more input information than in the case of independent input variables.

7.5 Mixed possibilistic and probabilistic approaches

Just for reference, Dubois (2006) mentions the works of Ferson and Ginzburg (1995), Guyonnet et al. (2003), and Baudrit et al. (2005) as recent proposals to solve the uncertainty propagation problem in cases in which some of the input variables are independent random variables and the others are possibilistic variables based on a common source of information, independent of the source(s) of information of the random variables. These authors apply a hybrid method of simulation of Monte Carlo (for the random variables) and fuzzy interval arithmetic (for the possibilistic variables) to obtain so-called upper and lower distribution functions for the output variable. However, it is acknowledged that both the (in)dependence relations among random and possibilistic variables, and the physical interpretation of the results require more research.

8 Conclusions

The following conclusions are highlighted:

1. On attaching a probability measure to an uncertain physical variable X, care should be taken in relating the "correct value" x^* of X with parameters of the probability distribution of X (e.g., mean μ or mode x_0) (Section 4, in fine).
2. Possibility and necessity measures are not independent but dual measures, i.e., they express the same uncertainty information in different ways (introduction of Section 5).
3. In Section 5.1, three methods are proposed to convert available probability uncertainty information on input variables (e.g., more or less reliable probability distributions, or point and interval estimates of the "correct values") into physically meaningful possibility uncertainty measures for the same variables, at the cost of losing more or less uncertainty information. On the construction of possibility measures directly from the physical non-deterministic experiments behind the uncertain estimation of input variables, there is still much to be done.
4. The uncertainty information conveyed by the possibility distribution π of an output variable Y consists in (Section 5.2): (1) the mode y_0, which is the best point estimate of the "correct value" y^* and (2) any α-cut ($\alpha\in[0,1]$), which can be roughly interpreted as a confidence interval for y^* with confidence level $\alpha'=1-\alpha$ but with amplitude that is usually much larger than the optimum. The former interpretations are still not easy to extend to variables Y with multimodal possibility distributions π (cf. Section A2.2, Electronic supplementary material), which, fortunately, are rare in practice.
5. When it is not possible to attach a probability measure to an input variable X in a fully consistent way, the only available uncertainty information are subjective estimates of largely ignorant experts or it is simply wished to spare computation time on solving the subsequent uncertainty propagation problem, X can be treated as a possibilistic or fuzzy variable (Section 6). The second cause (i.e., the limitation of probability theory to deal with states of large ignorance) still needs to be better understood.
6. Fuzzy interval arithmetic (FIA) is a computationally cheap way of solving the uncertainty propagation problem when the input variables are fuzzy. In Section 7.1, very efficient but more or less general closed forms of FIA are given specifically to perform the uncertainty analysis of LCI problems. However, although not supposed to be restrictive in most practical cases, a deep physical understanding of the fundamental limitations of FIA and also of some more specific limitations of its implementations (e.g., Heijungs and Tan 2010) is still lacking.
7. The classical way of solving the uncertainty propagation problem for random input variables through the algorithm of simulation of Monte Carlo can be used both for

independent and correlated input variables but, in the latter case, much more input information is required (Sections 7.2 and 7.4). The practical investigation of probabilistic correlations among input variables of LCI, both of their existence and of the means to get the additional uncertainty information required, is supposed to be still very incipient.

8. On solving the uncertainty propagation problem, the possibilistic approach is computationally much faster but affords also much poorer output uncertainty information than the probabilistic approach (Section 7.3). However, the natural possibilistic point estimate of the "correct value" of an output variable [cf. Conclusion 4, (1)] should also be adopted in the probabilistic approach.
9. There exist recent proposals to solve the uncertainty propagation problem through mixed possibilistic/probabilistic approaches when the set of input variables is composed both of random and fuzzy variables, but the physical interpretations of their conditions of application and output information are still deficient (Section 7.5).

Acknowledgments The first author is grateful to his colleague Prof. Fausto Freire for bringing to his knowledge and encourage the study of the seminal paper of Tan (2008).

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